ELSEVIER

Analytica Chimica Acta 446 (2001) 503–505

ANALYTICA CHIMICA ACTA

www.elsevier.com/locate/aca

Author Index

Alsberg, B.K.
—, Marchand-Geneste, N. and King, R.D.
Modeling quantitative structure–property relationships in calculated reaction pathways using a new 3D quantum topological representation 3

Bacci, M.
—, Fabbri, M., Picollo, M. and Porcinai, S.
Non-invasive fibre optic Fourier transform-infrared reflectance spectroscopy on painted layers. Identification of materials by means of principal component analysis and Mahalanobis distance 15
Barros, A., see Rutledge, D.N. 281
Batonneau, Y.
—, Laureyns, J., Merlin, J.-C. and Brémard, C.
Self-modeling mixture analysis of Raman microspectrometric investigations of dust emitted by lead and zinc smelters 23
Bloomfield, M.S., see Vannecke, C. 413
Boqué, R., see Maroto, A. 133
Bosch-Reig, F., see Tortajada-Genaro, L.A. 385
Boucon, C., see Guo, Q. 85
Brémard, C., see Batonneau, Y. 23
Bro, R., see Munck, L. 171
Bugelski, P.J., see Wu, W. 451
Buydens, L.M.C., see de Groot, P.J. 71
Buydens, L.M.C., see Kooistra, L. 97
Buydens, L.M.C., see Thissen, U. 371

Campíns-Falcó, P., see Tortajada-Genaro, L.A. 385
Cass, G.R., see Song, X.-H. 329
Coomber, T., see Vannecke, C. 413

da Costa Filho, P.A.
— and Poppi, R.J.
Determination of triglycerides in human plasma using near-infrared spectroscopy and multivariate calibration methods 39
de Groot, P.J.
—, Postma, G.J., Melssen, W.J., Buydens, L.M.C., Deckert, V. and Zenobi, R.
Application of principal component analysis to detect outliers and spectral deviations in near-field surface-enhanced Raman spectra 71
de Hoog, J., see Osán, J. 211
de Jong, S., see Guo, Q. 85
de Juan, A., see Navea, S. 187

De Spiegeleer, B.
—, Van Vooren, L., Voorspoels, J., Thoné, D. and Rosier, J.
Dissolution stability and IVIVC investigation of a buccal tablet 345
Deckert, V., see de Groot, P.J. 71
Delgadillo, I., see Rutledge, D.N. 281
Duponchel, L., see Ruckebusch, C. 257

Eberlin, M.N., see Zampronio, C.G. 495
Eide, I., see Shen, H. 313
Elcock, F.J., see Wu, W. 451
Engelsen, S.B., see Munck, L. 171
Esteban Díez, I., see Forina, M. 59

Fabbri, M., see Bacci, M. 15
Faber, N.M., see Song, X.-H. 329
Forina, M.
—, Lanteri, S. and Esteban Díez, I.
New index for clustering tendency 59
Funatsu, K., see Yoshida, H. 485

Gan, F., see Liang, Y. 115
Gargallo, R., see Vives, M. 439
Geladi, P., see Lindholm-Sethson, B. 121
Grung, B., see Shen, H. 313
Guo, Q.
—, Wu, W., Massart, D.L., Boucon, C. and de Jong, S.
Feature selection in sequential projection pursuit 85

Harrington, P.B., see Urbas, A.A. 393
Herrero, A., see Rueda, M.E. 269
Herrero, A., see Sanz, M.B. 297
Hopke, P.K., see Ramadan, Z. 233
Hopke, P.K., see Song, X.-H. 329
Huvenne, J.-P., see Ruckebusch, C. 257

Íñiguez, M., see Meléndez, M.E. 159

Jacobsen, S., see Munck, L. 171
Jacobsson, S.P., see Nord, L.I. 199
Javier del Río, F.
—, Riu, J. and F. Xavier Rius
Graphical criterion for the detection of outliers in linear regression taking into account errors in both axes 49
Jaworska, J., see Verdonck, F.A.M. 429

PII: S0003-2670(01)01449-0

Johnson, M.J., see Ramadan, Z. 233

Kenne, L., see Nord, L.I. 199
King, R.D., see Alsberg, B.K. 3
Kooistra, L.
—, Wehrens, R., Leuven, R.S.E.W. and Buydens, L.M.C.
Possibilities of visible–near-infrared spectroscopy for the assessment of soil contamination in river floodplains 97
Krawczyk, W.
— and Parczewski, A.
Application of chemometric methods in searching for illicit Leuckart amphetamine sources 107
Kvalheim, O.M., see Shen, H. 313

Lanteri, S., see Forina, M. 59
Laureyns, J., see Batonneau, Y. 23
Leardi, R., see Yoshida, H. 485
Leuven, R.S.E.W., see Kooistra, L. 97
Liang, Y.
— and Gan, F.
Chemical knowledge discovery from mass spectral database. I. Isotope distribution and Beynon table 115
Lindholm-Sethson, B.
—, Geladi, P. and Nelson, A.
Interaction with a phospholipid monolayer on a mercury electrode. Multivariate analysis of impedance data 121

Marchand-Geneste, N., see Alsberg, B.K. 3
Maroto, A.
—, Boqué, R., Riu, J. and Xavier Rius, F.
Estimation of measurement uncertainty by using regression techniques and spiked samples 133
Martínez, A.
—, Riu, J. and Xavier Rius, F.
Multiple analytical method comparison using maximum likelihood principal component analysis and linear regression with errors in both axes 147
Massart, D.L., see Guo, Q. 85
Massart, D.L., see Vannecke, C. 413
Masulli, F., see Pardo, M. 223
Meléndez, M.E.
—, Sánchez, M.S., Íñiguez, M., Sarabia, L.A. and Ortiz, M.C.
Psychophysical parameters of colour and the chemometric characterisation of wines of the certified denomination of origin 'Rioja' 159
Melssen, W.J., see de Groot, P.J. 71
Melssen, W.J., see Thissen, U. 371
Merlin, J.-C., see Batonneau, Y. 23
Mikedi, K., see Statheropoulos, M. 353
Møller, B., see Munck, L. 171
Moraes, L.A.B., see Zampronio, C.G. 495
Moreno, V., see Vives, M. 439
Munck, L.
—, Pram Nielsen, J., Møller, B., Jacobsen, S., Søndergaard, I., Engelsen, S.B., Nørgaard, L. and Bro, R.
Exploring the phenotypic expression of a regulatory proteome-altering gene by spectroscopy and chemometrics 171

Navea, S.
—, de Juan, A. and Tauler, R.
Three-way data analysis applied to multispectroscopic monitoring of protein folding 187
Nelson, A., see Lindholm-Sethson, B. 121
Nichols, W.F., see Windig, W. 467
Nord, L.I.
—, Kenne, L. and Jacobsson, S.P.
Multivariate analysis of ^{1}H NMR spectra for saponins from *Quillaja saponaria* Molina 199
Nørgaard, L., see Munck, L. 171

Oh, K.-Y., see Osán, J. 211
Ortiz, M.C., see Meléndez, M.E. 159
Ortiz, M.C., see Rueda, M.E. 269
Ortiz, M.C., see Sanz, M.B. 297
Osán, J.
—, de Hoog, J., Worobiec, A., Ro, C.-U., Oh, K.-Y., Szalóki, I. and Van Grieken, R.
Application of chemometric methods for classification of atmospheric particles based on thin-window electron probe microanalysis data 211

Parczewski, A., see Krawczyk, W. 107
Pardo, M.
—, Sberveglieri, G., Taroni, A., Masulli, F. and Valentini, G.
Decompositive classification models for electronic noses 223
Picollo, M., see Bacci, M. 15
Poppi, R.J., see da Costa Filho, P.A. 39
Poppi, R.J., see Zampronio, C.G. 495
Porcinai, S., see Bacci, M. 15
Postma, G.J., see de Groot, P.J. 71
Pram Nielsen, J., see Munck, L. 171
Prather, K.A., see Song, X.-H. 329

Ramadan, Z.
—, Song, X.-H., Hopke, P.K., Johnson, M.J. and Scow, K.M.
Variable selection in classification of environmental soil samples for partial least square and neural network models 233
Rambali, B., see Rousseeuw, P.J. 245
Riu, J., see Javier del Río, F. 49
Riu, J., see Maroto, A. 133
Riu, J., see Martínez, A. 147
Ro, C.-U., see Osán, J. 211
Rosier, J., see De Spiegeleer, B. 345
Rousseeuw, P.J.
—, Van Aelst, S., Rambali, B. and Smeyers-Verbeke, J.
Deepest regression in analytical chemistry 245
Ruckebusch, C.
—, Duponchel, L. and Huvenne, J.-P.
Degree of hydrolysis from mid-infrared spectra 257
Rueda, M.E.
—, Sarabia, L.A., Herrero, A. and Ortiz, M.C.
Soft calibration in a flow system with electrochemical detection. Application to the determination of phenolic compounds 269
Rutledge, D.N.
—, Barros, A. and Delgadillo, I.
PoLiSh — smoothed partial least-squares regression 281

Sánchez, M.S., see Meléndez, M.E. 159
Sanz, M.B.
—, Sarabia, L.A., Herrero, A. and Ortiz, M.C.
Capability of discrimination: application to soft calibration methods 297
Sarabia, L.A., see Meléndez, M.E. 159
Sarabia, L.A., see Rueda, M.E. 269
Sarabia, L.A., see Sanz, M.B. 297
Sberveglieri, G., see Pardo, M. 223
Schauer, J.J., see Song, X.-H. 329
Scow, K.M., see Ramadan, Z. 233
Shen, H.
—, Grung, B., Kvalheim, O.M. and Eide, I.
Automated curve resolution applied to data from multi-detection instruments 313
Smeyers-Verbeke, J., see Rousseeuw, P.J. 245
Smith, W.F., see Windig, W. 467
Søndergaard, I., see Munck, L. 171
Song, X.-H.
—, Faber, N.M., Hopke, P.K., Suess, D.T., Prather, K.A., Schauer, J.J. and Cass, G.R.
Source apportionment of gasoline and diesel by multivariate calibration based on single particle mass spectral data 329
Song, X.-H., see Ramadan, Z. 233
Statheropoulos, M.
— and Mikedi, K.
PCA–ContVarDia: an improvement of the PCA–VarDia technique for curve resolution in GC–MS and TG–MS analysis 353
Suess, D.T., see Song, X.-H. 329
Szalóki, I., see Osán, J. 211

Taroni, A., see Pardo, M. 223
Tauler, R., see Navea, S. 187
Tauler, R., see Vives, M. 439
Thas, O., see Verdonck, F.A.M. 429
Thissen, U.
—, Melssen, W.J. and Buydens, L.M.C.
Nonlinear process monitoring using bottle-neck neural networks 371
Thoné, D., see De Spiegeleer, B. 345
Tortajada-Genaro, L.A.
—, Campíns-Falcó, P. and Bosch-Reig, F.
Calibration transfer in chemiluminescence analysis. Application to chromium determination by luminol–hydrogen peroxide reaction 385

Urbas, A.A.
— and Harrington, P.B.
Two-dimensional wavelet compression of ion mobility spectra 393

Valentini, G., see Pardo, M. 223
Van Aelst, S., see Rousseeuw, P.J. 245
Van Grieken, R., see Osán, J. 211
Van Gyseghem, E., see Vannecke, C. 413
Van Vooren, L., see De Spiegeleer, B. 345
Vander Heyden, Y., see Vannecke, C. 413
Vannecke, C.
—, Van Gyseghem, E., Bloomfield, M.S., Coomber, T., Vander Heyden, Y. and Massart, D.L.
Development of a generic flow injection analysis method for compounds with a secondary amine or amide function, using an experimental design approach. I. Selection and evaluation of the FIA system parameters 413
Vanrolleghem, P.A., see Verdonck, F.A.M. 429
Varmuza, K., see Yoshida, H. 485
Verdonck, F.A.M.
—, Jaworska, J., Thas, O. and Vanrolleghem, P.A.
Determining environmental standards using bootstrapping, bayesian and maximum likelihood techniques: a comparative study 429
Vives, M.
—, Tauler, R., Moreno, V. and Gargallo, R.
Study of the interaction of a *cis*-dichloroaminopyrrolidine Pt(II) complex and the polynucleotide poly(I)–poly(C) acid by means of ^{1}H-NMR and multivariate curve resolution 439
Voorspoels, J., see De Spiegeleer, B. 345

Wehrens, R., see Kooistra, L. 97
Wildsmith, S.E., see Wu, W. 451
Windig, W.
—, Smith, W.F. and Nichols, W.F.
Fast interpretation of complex LC/MS data using chemometrics 467
Winkley, A.J., see Wu, W. 451
Worobiec, A., see Osán, J. 211
Wu, W., see Guo, Q. 85
Wu, W.
—, Wildsmith, S.E., Winkley, A.J., Yallop, R., Elcock, F.J. and Bugelski, P.J.
Chemometric strategies for normalisation of gene expression data obtained from cDNA microarrays 451

Xavier Rius, F., see del Río, F. Javier 49
Xavier Rius, F., see Maroto, A. 133
Xavier Rius, F., see Martínez, A. 147
Xu, L.
— and Zhang, W.-J.
Comparison of different methods for variable selection 477

Yallop, R., see Wu, W. 451
Yoshida, H.
—, Leardi, R., Funatsu, K. and Varmuza, K.
Feature selection by genetic algorithms for mass spectral classifiers 485

Zampronio, C.G.
—, Moraes, L.A.B., Eberlin, M.N. and Poppi, R.J.
Multivariate curve resolution applied to MS/MS data obtained from isomeric mixtures 495
Zenobi, R., see de Groot, P.J. 71
Zhang, W.-J., see Xu, L. 477